Sarcosine, N-(4-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C13H14F3NO3/c1-3-20-11(18)8-17(2)12(19)9-4-6-10(7-5-9)13(14,15)16/h4-7H

InchiKey: GTEZNVCNKBUBIE-UHFFFAOYSA-N

Formula: C13H14F3NO3

SMILES: CCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-672.29	kJ/mol	Joback Method
hf	-973.52	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.341		Crippen Method
mcvol	194.570	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	665.68	K	Joback Method
tc	859.37	K	Joback Method
tf	433.96	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.95	J/mol×K	665.68	Joback Method
cpg	540.06	J/mol×K	697.96	Joback Method
cpg	552.29	J/mol×K	730.24	Joback Method
cpg	563.69	J/mol×K	762.52	Joback Method
cpg	574.29	J/mol×K	794.80	Joback Method
cpg	584.14	J/mol×K	827.09	Joback Method
cpg	593.27	J/mol×K	859.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume